

Metallic behavior in Si/SiGe 2D electron systems

E. H. Hwang and S. Das Sarma

Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111
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We calculate the temperature, density, and parallel magnetic field dependence of low temperature electronic resistivity in 2D high-mobility Si/SiGe quantum structures, assuming the conductivity limiting mechanism to be carrier scattering by screened random charged Coulombic impurity centers. We obtain comprehensive agreement with existing experimental transport data, compellingly establishing that the observed 2D metallic behavior in low-density Si/SiGe systems arises from the peculiar nature of 2D screening of long-range impurity disorder. In particular, our theory correctly predicts the experimentally observed metallic temperature dependence of 2D resistivity in the fully spin-polarized system.

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The two-dimensional (2D) “metallicity” is by now a well-established ubiquitous low-temperature phenomena [1] where a relatively high-quality (i.e. low disorder) 2D carrier (either electron or hole) system confined in semiconductor heterostructures exhibits a pronounced temperature (T) and/or parallel (i.e. in the 2D plane) magnetic field (B_{\parallel}) dependent resistivity $\rho(T; B_{\parallel})$ in the dilute or low carrier density regime. The strength of the metallicity, i.e. the relative magnitude of the variation of $\rho(T)$ with T , is found to depend on the specific 2D material involved as also does the precise low-density regime where the strong metallicity manifests itself. For example, in 2D Si MOSFETs the metallicity occurs [2] around 10^{11}cm^{-2} with $\rho(T)$ changing by as much as a factor of 3 – 4 as temperature changes from 50 mK to 5K (at $B = 0$) whereas in 2D n-GaAs electron systems the metallicity is observed [3] for density well below 10^{10}cm^{-2} with $\rho(T)$ changing only by about 25% as T changes from 50 mK to a few K. The 2D metallicity has been experimentally observed in essentially all existing semiconductor-based 2D systems, most notable (and most extensively studied) being electrons in Si MOSFETs, holes in p-GaAs 2D structures [4] and very recently, electrons in n-GaAs 2D structures [3].

One of the more important systems to manifest 2D metallic behavior is the 2D electron system in modulation doped Si/SiGe structures [5–8] where the electrons are confined by the Si-SiGe interface potential barrier on the Si side of the heterostructure and the modulation doping delta layer (contributing the 2D electrons) is typically placed 100 – 200 Å inside the insulating SiGe side. The relatively impurity-free high quality of the materials (both Si and SiGe), and the lack of interface impurities and roughness (at the Si-SiGe interface) make the Si/SiGe 2D electron system essentially ideal from the perspective of understanding 2D metallic behavior. In particular, the dominant low-temperature (below 5K or so where phonon scattering should be exponentially suppressed in silicon) scattering mechanism in Si/SiGe 2D electron system is thought to be scattering by the remote dopants in the modulation delta layer

which, being far (i.e. 100 – 200 Å) away from the 2D electrons residing inside Si, leads to very high, by more than an order of magnitude higher than the corresponding Si MOSFETs, carrier mobilities. The high quality of the system and the simple isotropic parabolic 2D energy dispersion (in contrast to the p-GaAs based 2D hole systems which suffer from the multiband valence band structure, strong 2D anisotropy, strong spin-orbit coupling, inter-spin-split-band scattering, and strong phonon scattering leading to considerable complications in its 2D metallicity) make Si/SiGe based 2D electron systems an excellent candidate for studying 2D metallic behavior. In particular, 2D electrons in Si/SiGe structures combine, from the 2D metallic physics perspective, the advantages of n-Si MOSFETs (i.e. strong metallicity) with the advantages of the n-GaAs system (i.e., high mobility and low density) without the n-GaAs disadvantage of weak metallicity and phonon scattering problems. Metallicity has been observed [8] in 2D Si/SiGe systems down to densities as low as $3 \times 10^{10} \text{cm}^{-2}$, and the relevant interaction parameter (r_s) is typically 5 – 10 for this system.

In the context of 2D metallic physics it is therefore of considerable interest that recently two independent groups have reported detailed experimental data on the temperature, density, and parallel magnetic field dependence of 2D resistivity in Si/SiGe confined electron systems. The reported Si/SiGe experimental results, particularly in the presence of a parallel magnetic field, have significant *qualitative* difference with the corresponding experimental results in n-Si MOSFETs, warranting a theoretical investigation. We provide, in this Communication, such a transport theory for 2D electrons in Si/SiGe structures, finding good agreement between our theoretical and the existing experimental results.

We use a minimal zeroth-order theoretical model [9] to describe the 2D transport properties, keeping the total number of unknown parameters to a minimum. We neglect all phonon scattering effects although it is fairly straightforward to include them, mainly because our theoretical estimate shows phonon scattering to be negligible for 2D electrons in Si/SiGe structures in the $T < 5K$

regime of interest to us. We assume that the 2D carrier conductivity is entirely limited by screened impurity scattering, where the disorder arises from random background charged impurity centers (i.e. unintentional dopants) and the ionized dopants (randomly distributed) in the modulation dopant layer. The background unintentional impurity density is extremely low ($\sim 10^{14} \text{cm}^{-3}$, which is equivalent to a 2D density of 10^8cm^{-2}), as implied by the high achieved mobilities ($\sim 7 \times 10^5 \text{cm}^2/\text{Vs}$) in gated Si/SiGe quantum well structures. The 2D resistivity is given in the Boltzmann theory by $\rho = m/ne^2\langle\tau\rangle$, where n , m , τ are respectively the 2D carrier density, the carrier effective mass, the transport relaxation time, and

$$\langle\tau\rangle = \int d\epsilon \epsilon \tau(\epsilon) \left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) / \int d\epsilon \left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right), \quad (1)$$

with $f(\epsilon)$ being the Fermi distribution function and

$$\frac{1}{\tau(\epsilon_{\mathbf{k}})} = \frac{2\pi}{\hbar} \int dz \int \frac{d^2 k'}{(2\pi)^2} N_i(z) |u^{e-i}(\mathbf{k} - \mathbf{k}', z)|^2 \times (1 - \cos \theta_{\mathbf{k}\mathbf{k}'}) \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}). \quad (2)$$

Eq. (1) indicates a thermal average over the energy dependent relaxation time $\tau(\epsilon)$, with $\epsilon = k^2/2m$ being the usual parabolic 2D electron energy dispersion. In Eq. (2), $u^{e-i}(q; z)$ is the (finite-temperature) screened electron-impurity interaction for 2D momentum transfer of q and $N_i(z)$ is the random charged impurity density in the direction (z) normal to the 2D (x - y) plane of confinement of the electron layer (the $z = 0$ being the Si/SiGe interface plane), which is given in our model by $N_i(z) = N_i^{3D} + n_i \delta(z - z_i)$, where N_i^{3D} is the background 3D charged impurity density and n_i is the 2D charged dopant density in the modulation doping δ -layer at $z = z_i$. We take z_i to coincide with the modulation doping layer in the experimental Si/SiGe samples. The key quantity in Eqs. (1)–(2) is the screened charged impurity disorder potential u^{e-i} , which we take to be

$$u^{e-i}(q, z) = v^{e-i}(q; z)/\epsilon(q), \quad (3)$$

where v^{e-i} is the bare Coulomb potential for electron-charged impurity interaction, and $\epsilon(q) = 1 - v(q)\Pi(q)$ is the RPA dielectric screening function due to the 2D electrons themselves, where $v(q)$ is the 2D bare Coulomb electron-electron interaction, and $\Pi(q) \equiv \Pi(q; T)$ is the 2D finite-temperature and finite wave vector polarizability function. All our calculations include the realistic quasi-2D quantum form factor effects, arising from the finite width of the 2D layer in z -direction, which enter the expressions for $v(q)$ and $v^{e-i}(q)$, that are of considerable quantitative importance. All quantities entering the theory are known except for N_i^{3D} and n_i , which are the only two parameters of the model. We set $N_i = 2 \times 10^{14} \text{cm}^{-3}$, $n_i = 3.5 \times 10^{10} \text{cm}^{-2}$, $z_i = 100 \text{\AA}$ throughout our calculations, instead of using them as adjustable parameters

since our interest here is a qualitative (and perhaps semi-quantitative) understanding of 2D metallicity in Si/SiGe systems. Note that there is little scattering by interface impurities and interface roughness in high-mobility Si/SiGe 2D systems, which is their distinguishing feature compared with Si MOS systems, leading to the extraordinarily (a factor of 20 – 40 higher than in Si MOSFETs) high 2D mobility.

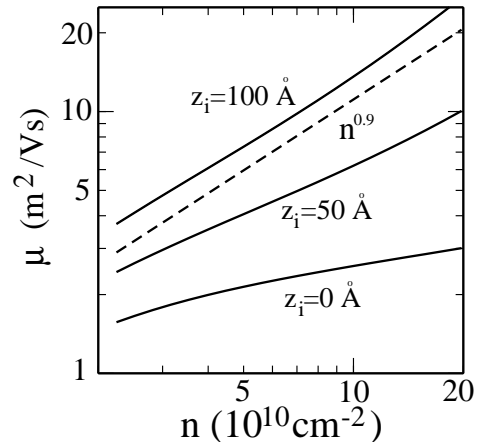


FIG. 1. The calculated 2D mobility of Si/SiGe 2D systems at 0.3K as a function of carrier density for different values of z_i . Dashed line represents $\mu \propto n^{0.9}$.

In Fig. 1 we show our calculated 2D mobility, $\mu = 1/ne\rho$, as a function of 2D electron density at $T = 0.3\text{K}$ for a number of different values of z_i , the position of the 2D dopant layer. The calculated mobility for $z_i = 100 \text{\AA}$ agrees well (quantitatively for $n > 0.5 \times 10^{11} \text{cm}^{-2}$) with the density-dependent mobility measured experimentally [8] which also (in agreement with Fig. 1) manifests a $\mu \propto n^{0.9}$ dependence on density at higher densities in contrast to $\mu \propto n^{0.3}$ behavior observed in Si MOSFETs (i.e., our $z_i = 0$ result corresponding to scattering by interface impurities). This establishes the validity of our model for the experimental Si/SiGe 2D systems.

In Fig. 2 – 4 we show our calculated results for the 2D resistivity in Si/SiGe systems. In Fig. 2 we show the zero-field ($B_{\parallel} = 0$) temperature dependence of the 2D resistivity for a number of carrier densities in the 2D metallic phase. The theoretical results are in excellent qualitative agreement with experimental observations [5–8] with the maximum temperature induced fractional change in the resistivity, $\Delta\rho/\rho_0$ where $\rho = \rho_0 + \Delta\rho(T)$ with $\rho_0 = \rho(T \rightarrow 0)$, being about 2 at lower densities in the $T \approx 100\text{mK} - 5\text{K}$ range. At higher densities ($> 10^{11} \text{cm}^{-2}$), $\Delta\rho/\Delta_0$ is, consistent with the experimental data, only about 50% (in the 0 – 5K range). The relatively weaker temperature dependence in Si/SiGe 2D system compared with Si MOS system arises entirely from the suppressed role of $2k_F$ -scattering in the modulation doped Si/SiGe systems – in fact, the

Si/SiGe system will manifest very strong (stronger than Si MOSFET) 2D metallicity if its mobility would be limited by interface scattering as in Si MOSFETs (or purely by the background impurities as in p-GaAs and n-GaAs 2D systems). It is well-known that the strong metallicity in the transport properties of low-disorder 2D systems arises from the temperature induced suppression of the $2k_F$ -Kohn anomaly in screening (i.e. the $T = 0$ cusp at $q = 2k_F$ in the 2D polarizability function), and the overall strong suppression of $2k_F$ scattering in the modulation doped structures [due to the presence of the $e^{-2k_F|z|}$ factor in the electron-impurity bare interaction $v^{e-i}(q; z)$ in Eq. (3)] leads to relatively weaker 2D metallicity. In fact, the temperature dependence would be substantially weaker than that in Fig. 2 (and therefore substantially weaker than the experimental observation) if we set the background impurity density N_i^{3D} to be zero in our calculation. The temperature dependence (Fig. 2) of $\rho(T; n)$ is thus a simple diagnostic for the strength of background impurity scattering in Si/SiGe system just as the density dependence (Fig. 1) is a diagnostic for the remote impurity scattering. We also mention the “almost parallel” behavior of $\rho(T)$ at various densities in Fig. 2, which has been experimentally seen [8].

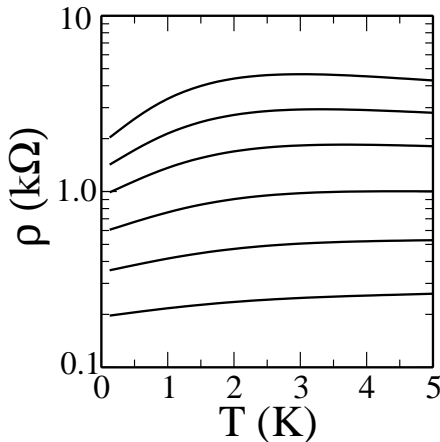


FIG. 2. Calculated resistivity as a function of temperature, $\rho(T)$, of 2D Si/SiGe systems for various densities $n = 4.2, 5.15, 6.3, 8.2, 10.8, 14.5 \times 10^{10} \text{ cm}^{-2}$ (top to bottom).

In Fig. 2 $\rho(T)$ shows a nonmonotonicity (particularly prominent at lower densities) where it increases with T at first and then decreases with increasing T after going through a shallow maximum at a characteristic density-dependent temperature $T_p(n)$ where $d\rho/dT$ changes sign, i.e. $d\rho/dT = 0$ at $T = T_p$. Our theoretical $T_p(n)$ in Fig. 2 scales approximately with the Fermi temperature T_F , but is not identical to T_F . This is precisely the experimental observation [8]. This non-monotonicity, which is obviously a non-asymptotic finite temperature phenomenon, arises from the competition between an increasing and decreasing contribution to $\rho(T)$ as defined by Eqs. (1)

– (3). The temperature dependence of the dielectric screening function in Eq. (3), with screening (particularly the strongly resistive $2k_F$ -scattering) decreasing with increasing temperature, gives rise to increasing effective disorder with increasing T , and hence increasing $\rho(T)$ with T . At higher temperatures the thermal averaging in Eq. (1), which always leads to $\rho(T)$ decreasing with T , becomes quantitatively more important, giving rise eventually to a $\rho(T)$ decreasing with T for $T > T_p$. In the classical non-degenerate regime the thermal averaging *always* wins out and impurity scattering limited $\rho(T)$ necessarily decreases with increasing T (which is why we earlier called this nonmonotonicity somewhat simplistically “the quantum-classical crossover”, generating some confusion on this matter), but thermal averaging *always* (i.e. even in the quantum $T \ll T_F$ regime) leads to a negative sub-leading contribution to $\rho(T)$ going as $O(T/T_F)^2$, whereas the screening contributes the leading order term going as $O(T/T_F)$, so in the $T/T_F \rightarrow 0$ limit the increasing contribution arising from $2k_F$ screening wins out. Depending on the details of the system, $T_p(n)$ could be quite low (e.g. much lower than T_F in weakly screening systems) although it should scale approximately with T_F . Our theoretical $T_p(n)$ in Fig. 2 is roughly of the order of the experimental T_p , but the theoretical T_p is somewhat higher quantitatively than the experimental T_p . Many details (e.g. phonon scattering, exact charged impurity distribution, the confinement potential, the effective mass, etc.) affect the precise value of T_p , and therefore a quantitative comparison between theory and experiment is not particularly meaningful.

In Figs. 3 and 4 we show our calculated results for the 2D magnetoresistance in Si/SiGe system in the presence of a parallel magnetic field B_{\parallel} which polarizes electron spins, consequently weakening screening considerably (i.e. B_{\parallel} acts similar to finite T effects). Of the three physical mechanisms [10] that affect 2D parallel field magnetoresistance, we have ignored the magneto-orbit effect [11] because it is negligibly small in the Si system at the applied parallel field values of experimental interest. We include the other two (competing) parallel field corrections, both arising from the electronic spin polarization induced by the applied field (and therefore both saturating for $B_{\parallel} \geq B_c$ where the system is completely spin polarized) — these being the spin-polarization induced weakening of screening (leading to positive magnetoresistance) and the spin-polarization induced enhancement of the 2D Fermi wave vector k_F (leading to negative magnetoresistance). The Si 2D system of interest to us is a strongly screening system with $q_{TF}/2k_F \gg 1$, where q_{TF} is the 2D screening wave vector, and therefore the screening effect is by far the dominant parallel field effect, producing a strong positive magnetoresistance apparent in Figs. 3 and 4 (and in the experiments).

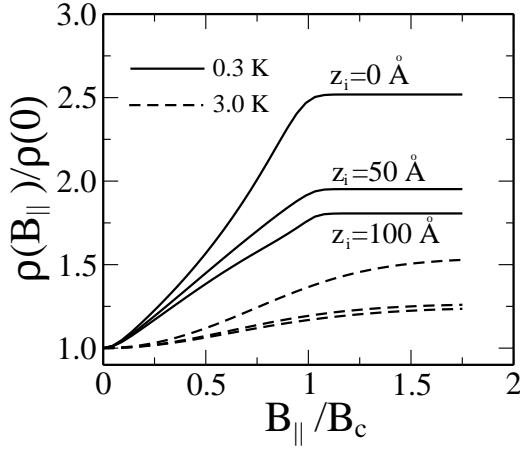


FIG. 3. Calculated magnetoresistance as a function of in-plane magnetic field for different values of the impurity separation $z_i = 0, 50, 100 \text{ \AA}$ at a fixed 2D density $n = 10^{11} \text{ cm}^{-2}$ and at $T = 0.3 \text{ K}$ (solid lines) and 3.0 K (dashed lines).

In Fig. 3 we show the calculated magnetoresistance $\rho(B_{||})/\rho(0)$ for different values of the impurity separation z_i . As expected, larger values of z_i drastically reduce the maximum magnetoresistance since the separation between the impurities and the 2D electrons suppresses the quantitative importance of $2k_F$ resistive scattering. Our maximum theoretical value of $\rho(B_{||})/\rho(0)$ for $z_i = 100 \text{ \AA}$ of about 1.7 is in excellent agreement with the corresponding experimentally observed [8] value, lending support to our theoretical screening picture.

In Fig. 4, which is perhaps the most important result presented in this work, we show our calculated magnetoresistance as a function of $B_{||}$ (at a fixed 2D density of 10^{11} cm^{-2}) for several different temperatures – the inset of Fig. 4 shows $\rho(T)$ at $B_{||} = 0$ and 9 T ($> B_c \approx 5 \text{ T}$ at 10^{11} cm^{-2} density). The theoretical results in Fig. 4 are qualitatively similar to the corresponding experimental results. The most important feature of Fig. 4 is the metallic temperature dependence of $\rho(T; B_{||})$ at $B_{||} > B_c$, which, although suppressed from the strong zero-field metallic temperature dependence $\rho(T; B_{||} = 0)$ due to the spin-polarization induced suppression of screening as the spin degeneracy changes from the paramagnetic value of 2 for $B_{||} = 0$ to the “ferromagnetic” value of 1 for $B_{||} \geq B_c$, is still strongly metallic in character with $\rho(T)$ changing by almost 50 % at $B_{||} = 9 \text{ T} \approx 2B_c$. This is precisely the experimental observation. In fact, our calculated temperature dependence of $\rho(T; B_{||} > B_c)$ is in excellent qualitative agreement with the experimental results [7].

The significance of our theoretical agreement with the observed “metallic” (i.e. $d\rho/dT > 0$) resistivity for $B_{||} > B_c$ arises from the very specific and contrasting prediction for $\rho(T; B_{||} > B_c)$ in the so-called “interaction theory” [12], which purports to extend the screening theory by calculating the electron-electron interaction effects

(to leading order in T/T_F) on the 2D transport properties to *all order* (perturbatively) in interaction for an unrealistic zero-range white-noise model of bare impurity disorder. The categorical prediction [12] of the interaction theory is that for a fully spin polarized 2D system (i.e. for $B_{||} \geq B_c$) the 2D resistivity must necessarily manifest an “insulating” (i.e., $d\rho/dT < 0$ for $B_{||} > B_c$) behavior. This interaction theory prediction obviously disagrees qualitatively with our results in Fig. 4, where $d\rho/dT > 0$ for $B_{||} > B_c$, as well as with experimental observations [7] in the Si/SiGe based high-mobility 2D electron systems. This qualitative disagreement (agreement) between interaction (screening) theory and experiment shows that the interaction theory is invalid in the 2D Si/SiGe systems due to the long-range nature of the underlying impurity disorder. We have also calculated (not shown) $\rho(B_{||})$ as a function of $B_{||}$ at various densities, finding that $\rho(B_{||})/\rho(0)$ at various densities approximately scale with $B_{||}/B_c$ as reported experimentally [8]. But we find that this scaling is non-universal and somewhat temperature dependent.

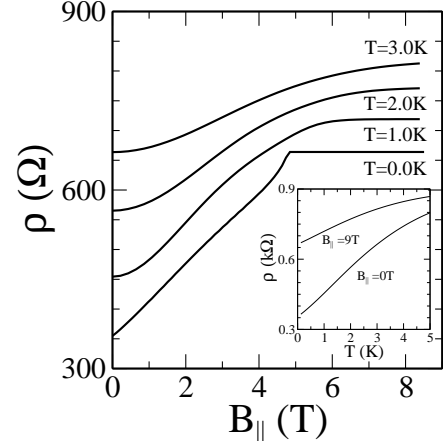


FIG. 4. Calculated magnetoresistance as a function of in-plane magnetic field for different temperatures at a fixed carrier density $n = 10^{11} \text{ cm}^{-2}$. Inset shows the resistivities $\rho(T, B_{||})$ at $B_{||} = 0$ and 9 T as a function of temperature.

In summary, we have developed a realistic screening theory for the density, temperature, and parallel magnetic field dependence of low-temperature 2D resistivity $\rho(T; n; B_{||})$ in Si/SiGe electron systems. Our results are in comprehensive qualitative agreement (in T , n , and $B_{||}$ dependence) with recent experimental observations [5–8]. In particular, we get agreement with the experimental observation of a “metallic” (i.e., $d\rho/dT > 0$) 2D resistivity in the completely spin-polarized ($B_{||} > B_c$) system, which disagrees qualitatively with the opposite prediction (i.e. $d\rho/dT < 0$ for $B_{||} > B_c$) of the interaction theory [12]. The agreement between our theory and experiments directly demonstrates the key role of long-range Coulombic disorder in 2D metallicity.

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